Exponential number of stationary solutions for Nagumo equations on graphs

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Abstract

We study the Nagumo reaction-diffusion equation on graphs and its dependence on the underlying graph structure and reaction-diffusion parameters. We provide necessary and sufficient conditions for the existence and nonexistence of spatially heterogeneous stationary solutions. Furthermore, we observe that for sufficiently strong reactions (or sufficiently weak diffusion) there are 3^n stationary solutions out of which 2^n are asymptotically stable. Our analysis reveals interesting relationship between the analytic properties (diffusion and reaction parameters) and various graph characteristics (degree distribution, graph diameter, eigenvalues). We illustrate our results by a detailed analysis of the Nagumo equation on a simple graph and conclude with a list of open questions.

Keywords: reaction-diffusion equation; graphs; graph Laplacian; variational methods; bifurcations

MSC 2010 subject classification: 34A33, 35K57

1 Introduction

The classical reaction-diffusion equation (also called the KPP equation)

$$\partial_t u(x,t) = d\partial_{xx}u(x,t) + \lambda f(u(x,t)), \quad d>0,\ \lambda>0,\ x\in\Omega\in\mathbb{R}^n,\ t>0, \tag{1.1}$$

is an influential nonlinear partial differential equation describing the evolution of chemical concentrations, temperatures, or populations. These phenomena combine a local dynamics (via the reaction function f) and a spatial dynamics (via the diffusion). It is well known that solutions to reaction-diffusion systems can exhibit rich behavior, e.g., the existence of traveling waves, pattern formation etc. [29].

However, in many situations, the continuous domains do not correspond to the real-world phenomena like population dynamics, neuron transmissions, image processing etc. [3, 9, 13, 14]. Consequently, various authors have considered the lattice reaction-diffusion equation [7, 8, 30, 31]

$$\partial_t u(x,t) = d(u(x+1,t) - 2u(x,t) + u(x-1,t)) + \lambda f(u(x,t)), \quad x\in\mathbb{Z}, \quad t\in[0,\infty), \tag{1.2}$$

or the discrete-time lattice reaction-diffusion equation (the so-called coupled map lattices) [5, 8]

$$u(x,t+1) - u(x,t) = d(u(x+1,t) - 2u(x,t) + u(x-1,t)) + \lambda f(u(x,t)), \quad x\in\mathbb{Z}, \quad t\in\mathbb{N}_0. \tag{1.3}$$

Obviously, equations (1.2) and (1.3) are also interesting from the standpoint of numerical mathematics. We can get (1.2) by a partial finite-difference approximation of (1.1) (method of lines) and (1.3) could be obtained by a full finite-difference approximation of (1.1).

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Keener [13] was the first one to establish that the dynamic behaviour of (1.1) and (1.2) is strikingly different. Whereas (1.1) has a travelling wave solutions for any $d > 0$, the problem (1.2) with sufficiently small $d > 0$ has infinite number of stable standing wave solutions implying the failure of propagation for all initial conditions. Similarly, Chow and Shen [5] studied this phenomenon, the spatial topological chaos, for the discrete time model (1.3). Many papers followed their footsteps, e.g. [6, 7, 8, 12, 16, 30, 31].

In this paper, we take a slightly different approach by considering finite but heterogeneous underlying discrete structures, undirected graphs. Arguably, both habitats in population models as well as the cell networks in cell transmission models form finite and irregular graphs structures (in contrast to regular infinite lattices as implied by the models of the form (1.2)-(1.3)). This generalization follows a recent trend of studying dynamical systems on general networks, e.g., [21, 24].

In the context of dynamical systems on graph structures, we can distinguish between two distinct approaches. On the one hand, models with partial differential equations on each edge with vertices serving as connecting boundary points have been considered (e.g., [2, 4, 21]). On the other hand, the above approach (in which the unknown quantities are defined only in vertices and edges represent dependencies) makes sense from the numerical point of view [5, 6, 7, 8] but also in applications, e.g., in biology [1, 13] or image processing [14]. We follow this latter setting.

Let $G = (V, E)$ be a connected undirected graph with $V = \{1, 2, \dots, n\}$ being a set of vertices with $n = |V|$ and E a set of edges. We consider a reaction-diffusion equation on graphs

$$\partial_t u_i(t) = d \sum_{j \in N(i)} (u_j(t) - u_i(t)) + \lambda f(u_i(t)), \quad i \in V, \quad t \in [0, \infty), \tag{1.4}$$

where $d, \lambda > 0$ and $N(i) = \{j \in V : (i, j) \in E\}$ denotes the neighbourhood of $i \in V$. If we allow for different diffusion coefficients along the edges, our model becomes

$$\partial_t u_i(t) = \sum_{j \in N(i)} d_{ij}(u_j(t) - u_i(t)) + \lambda f(u_i(t)), \quad i \in V, \quad t \in [0, \infty), \tag{1.5}$$

where $d_{ij} > 0$. Alternatively, the sum in (1.5) could be taken over all vertices $j \in V$, $j \neq i$ and we could assume $d_{ij} \geq 0$ with $d_{ij} = 0$ when $(i, j) \notin E$. We only consider the symmetrical case $d_{ij} = d_{ji}$.

Two most common reaction functions (arising in population models) are the logistic growth/monostable reaction $f(u) = u(1 - u)$ (leading to the so-called Fisher reaction-diffusion equation) and the Allee effect/bistable reaction function $f(u) = u(u - a)(1 - u)$ (leading to the so-called Nagumo reaction-diffusion equation). We only focus on the latter nonlinearity and assume throughout the paper

(H_1) $f(s) = s(s - a)(1 - s)$ with $a \in (0, 1)$,

(H_2) $u_i(0) \in [0, 1]$ for all $i \in V$.

In Section 2 we provide an abstract formulation of (1.5) in $\mathbb{R}^n$ using the graph Laplacian matrix and study the constant solutions of (1.5) and their stability. Our main interest, though, is directed to the spatially heterogeneous (non-constant) stationary solutions. In Section 3 we provide some a priori estimates, show that for sufficiently small λ's there are no non-constant stationary solutions of (1.5) and provide sufficient conditions for the existence of non-constant stationary solutions. In Section 4 we show that for large λ's there are 3^n stationary solutions of (1.5) out of which 2^n are asymptotically stable. To illustrate our results we provide a simple example on a trivial graph $G = K_2$ in Section 5. This example and numerical results indicate that our results could be improved and thus we conclude with a set of open problems in Section 6.

In other words, our results show that for a fixed graph G and diffusion parameters d_{ij} we can define $\underline{\lambda}$ to be the infimum of all λ's such that the problem (1.5) has a non-constant stationary solutions and, similarly, $\overline{\lambda}$ to be the infimum of all λ's such that the problem (1.5) has 3^n non-constant stationary solutions (see Figure 1). Our results in Sections 3-4 could be understood as bounds for $\underline{\lambda}$ and $\overline{\lambda}$.

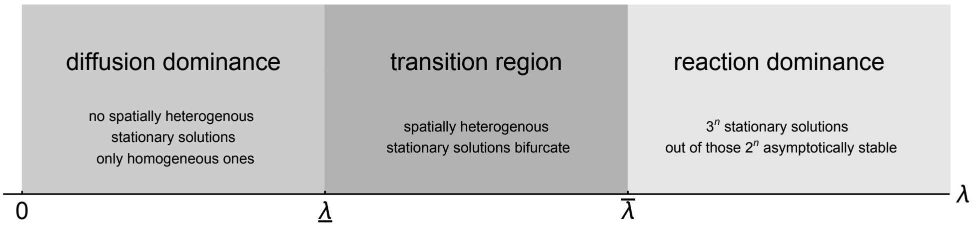


Figure 1: Existence of spatially heterogeneous (non-constant) stationary solutions of (1.5) in dependence on λ.

2 Abstract formulation and preliminaries

If we define the vector function $u(t) = [u_1(t), \dots, u_n(t)]$ we can rewrite (1.5) as

$$\partial_t u(t) = -Au(t) + \lambda F(u(t)), \tag{2.1}$$

where A is the $n \times n$ symmetric matrix,

$$A = \begin{bmatrix} \sum_{j\in N(1)} d_{1j} & -d_{12} & -d_{13} & \dots & -d_{1n} \\ -d_{21} & \sum_{j\in N(2)} d_{2j} & -d_{23} & \dots & -d_{2n} \\ -d_{31} & -d_{32} & \sum_{j\in N(3)} d_{3j} & \dots & -d_{3n} \\ \dots & \dots & \dots & \ddots & \dots \\ -d_{n1} & -d_{n2} & -d_{n3} & \dots & \sum_{j\in N(n)} d_{nj} \end{bmatrix},$$

with $d_{ij} > 0$ if and only if $(i, j) \in E$ (see Figure 2) and $F : \mathbb{R}^n \to \mathbb{R}^n$ is defined by

$$F(u) := \begin{bmatrix} f(u_1) \\ f(u_2) \\ \vdots \\ f(u_n) \end{bmatrix}.$$

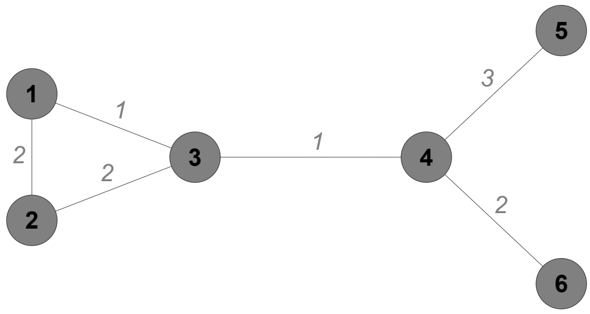
The matrix A is also known, especially in the graph-theoretical literature, as the graph Laplacian matrix [18] and is often denoted by $L(G)$ or, in the case of edge-weighted graphs, by $L(G_C)$ (we stick to the shorter notation A). The properties of its eigenvalues and their relationship to the graph theoretical characteristics have been studied by many authors, especially in the situation with $d_{ij} = 1$ for all $(i, j) \in E$. It is well-known that this matrix is positive semi-definite and $\lambda_1 = 0$ is the simple (if G is connected) eigenvalue with the corresponding eigenvector $e_1 = [1, 1, \dots, 1]$.

Since we only consider finite graphs, we are able to prove easily the uniqueness and invariance of the interval $[0, 1]$ for solutions of (1.5).

Theorem 2.1. *Under the assumptions* (H_1)-(H_2) *there exists a unique solution of the graph reaction-diffusion equation* (1.5)*. Moreover* $u_i(t) \in [0, 1]$*, with* $i \in V$*.*

Proof. The proof is a simple extension of [27, Theorem 18] and is thus omitted. $\square$

Remark 2.2. One of our goals is to connect the properties of (1.4)-(1.5) to those of the graph Laplacian A. This leads to the seemingly awkward use of $-A$ instead of the unsigned A in (2.1). The following section also shows that this choice is reasonable since it leads naturally to positive definite operators and coercive functionals. Similarly, we do not respect the usual procedure in the literature and fix d and study dependence of (1.4)-(1.5) on $\lambda > 0$. The main reason is that we allow for d to be non-constant along the edges, see (1.5).



$$A = \begin{pmatrix} 3 & -2 & -1 & 0 & 0 & 0 \\ -2 & 4 & -2 & 0 & 0 & 0 \\ -1 & -2 & 4 & -1 & 0 & 0 \\ 0 & 0 & -1 & 6 & -3 & -2 \\ 0 & 0 & 0 & -3 & 3 & 0 \\ 0 & 0 & 0 & -2 & 0 & 2 \end{pmatrix}$$

Figure 2: An example of a graph on 6 vertices with weights d_{ij} (indicated by gray numbers along the edges) and the corresponding graph Laplacian matrix A.

Throughout the paper we study stationary solutions of (1.5) and their stability . Considering (2.1) they straightforwardly satisfy the nonlinear algebraic equation in $\mathbb{R}^n$

$$o = -Au + \lambda F(u). \tag{2.2}$$

We immediately observe that all zeros of f provide constant (spatially homogeneous) solutions (since both $Au = o$ and $F(u) = o$). In the case of the bistable nonlinearity (H_1) this implies three constant stationary solutions

$$v^1(t) = o, \quad v^2(t) = ae_1 = [a, \dots, a] \quad v^3(t) = e_1 = [1, \dots, 1]. \tag{2.3}$$

For stationary solutions of (2.1) to be asymptotically stable it is sufficient to show that the eigenvalues of $-A + \lambda F'(u)$ have negative real parts. Given the properties of the graph Laplacian A and the fact that $\lambda F'(u)$ is a diagonal matrix with the following structure

$$\lambda F'(u) = \lambda \mathrm{diag}[(2 - 3u_1)u_1 + a(2u_1 - 1), \dots, (2 - 3u_n)u_n + a(2u_n - 1)],$$

we can immediately obtain the stability of constant solutions (2.3).

Theorem 2.3. *The constant stationary solutions of* (2.1) $v^1(t) = o$, *and* $v^3(t) = e_1$ *are asymptotically stable. The constant stationary solution* $v^2(t) = ae_1$ *is unstable.*

Proof. First, we observe $-A + \lambda F'(v^1) = -A + \mathrm{diag}[-\lambda a, \dots, -\lambda a]$. Since $-\lambda a < 0$ and A is positive semidefinite, we get that $-A + \lambda F'(v^1)$ is negative definite.

Similarly,

$$-A + \lambda F'(v^3) = -A + \mathrm{diag}[-\lambda(1 - a), \dots, -\lambda(1 - a)],$$

and we arrive to the same conclusion for v^3 based on the fact that $-\lambda(1 - a) < 0$.

In the same spirit, we get

$$-A + \lambda F'(v^2) = -A + \mathrm{diag}[\lambda(1 - a)a, \dots, \lambda(1 - a)a]$$

Since $\lambda(1 - a)a > 0$ and A is positive semidefinite, we observe that $-A + \lambda F'(v^2)$ is either indefinite or positive semidefinite, i.e., it has at least one positive eigenvalue. $\square$

3 Existence and nonexistence of non-constant stationary solutions

The structure of constant (spatially homogeneous) stationary solutions is rather trivial. For any $\lambda > 0$ there are 3 constant solutions, out of which 2 are asymptotically stable (see Theorem 2.3). On the other hand, the structure of non-constant (spatially heterogeneous) stationary solutions is complicated, their number and stability changes with λ and the graph properties. In this section we provide sufficient conditions for the existence and nonexistence of non-constant stationary solutions. First, we present a simple a priori estimate that shows that all entries of all stationary solutions of (1.5) are located in $[0, 1]$.

Lemma 3.1. *Let $u \in \mathbb{R}^n$ be a solution of* (2.2)*, then $u_i \in [0, 1]$ for all $i \in V$.*

Proof. Let us consider, by contradiction, that there exists $i_1 \in V$ with $u_{i_1} > 1$. Then the equality

$$\sum_{j \in N(i_1)} d_{i_1 j}(u_j - u_{i_1}) + \lambda f(u_{i_1}) = 0$$

together with the fact $f(u_{i_1}) < 0$ imply that there must be $i_2 \in N(i_1)$ such that $u_{i_2} > u_{i_1}$, because otherwise

$$\sum_{j \in N(i_1)} d_{i_1 j}(u_j - u_{i_1}) + \lambda f(u_{i_1}) < \sum_{j \in N(i_1)} d_{i_1 j}(u_j - u_{i_1}) \leq 0.$$

Using the same argument for i_2 we deduce that there exist $i_3 \in V$ such that $u_{i_3} > u_{i_2}$ and, similarly, a sequence i_k, $k \in \mathbb{N}$ such that $u_{i_k} > u_{i_{k-1}}$, a contradiction, since we have the finite number of vertices. Consequently, $u_i \leq 1$ for all $i \in V$.

Using the fact that $f(s) > 0$ for $s < 0$, the same argument could be repeated to show that $u_i \geq 0$. □

Moreover, the entries of non-constant stationary solutions must be localized both in $[0, a)$ and $(a, 1]$.

Lemma 3.2. *Let $u \in \mathbb{R}^n$ be a non-constant (spatially heterogeneous) solution of* (2.2)*, then there exists $i \in V$ with $u_i \in [0, a)$ and $j \in V$ with $u_j \in (a, 1]$.*

Proof. Lemma 3.1 implies that $u_i \in [0, 1]$ for all $i \in V$. Let us assume, by contradiction, that $u_i \geq a$ for all $i \in V$ (the case $u_i \leq a$ is similar and thus omitted). Then there exists $\underline{i} \in V$ such that $a \leq u_{\underline{i}} \leq u_i$ for all $i \in V$. Since $f(u_{\underline{i}}) \geq 0$, we have

$$0 = \sum_{j \in N(\underline{i})} d_{\underline{i}j} \left(u_j - u_{\underline{i}}\right) + \lambda f(u_{\underline{i}}) \geq 0,$$

and consequently, this implies that $a = u_{\underline{i}} = u_j$ for all $j \in N(u_{\underline{i}})$. Repeating the argument for all $j \in N(u_{\underline{i}})$ and so on we get that $a = u_i$ for all $i \in V$, a contradiction with u being a non-constant solution. □

If λ is sufficiently small we show that there are no non-constant stationary solutions. We denote by $\operatorname{diam}(G) = \max_{i,j \in V} \operatorname{dist}(i, j)$ the graph diameter, i.e. the length of a greatest of all shortest paths connecting any two vertices, by $d_{\min} = \min_{\{i,j\} \in E} d_{ij}$ and $d_{\max} = \max_{\{i,j\} \in E} d_{ij}$ the minimal and maximal diffusion coefficients along the edges of the graph and by $\Delta(G) = \max_{i \in V} \deg(i)$ the maximal degree among all vertices of G.

Theorem 3.3. *Let*

$$\lambda < \begin{cases} \dfrac{d_{\min}}{a(1-a)} & \text{if } \operatorname{diam}(G) = 1, \\[2ex] \dfrac{d_{\max}(\Delta(G) - 1)}{a(1-a)\left(\left(\frac{d_{\max}}{d_{\min}}(\Delta(G) - 1) + 1\right)^{\operatorname{diam}(G)-1} - 1\right)} & \text{if } \operatorname{diam}(G) > 1. \end{cases} \tag{3.1}$$

Then there exist no non-constant (spatially heterogeneous) stationary solutions of (1.5).

Proof. Let us assume, by contradiction, that $u \in \mathbb{R}^n$ is a non-constant stationary solution of (1.5). We divide the proof into two parts.

First, we assume that $a \geq \frac{1}{2}$. Lemma 3.2 yields that there exists $i_1 \in V$ such that $u_{i_1} \geq u_i$ for all $i \in V$ and $u_{i_1} = a + \varepsilon$ for some $\varepsilon > 0$. Since $f(s)$ is concave on $(a, 1)$ we have that for $s \in (a, 1)$

$$f(s) \leq f'(a)(s-a) = a(1-a)(s-a).$$

Consequently we have

$$0 = \sum_{j \in N(i_1)} d_{i_1 j}\,(u_j - u_{i_1}) + \lambda f(u_{i_1}) \leq \sum_{j \in N(i_1)} d_{i_1 j}\,(u_j - u_{i_1}) + \lambda a(1-a)(u_{i_1} - a).$$

Let $i_2 \in N(i_1)$ be such that $u_{i_2} \leq u_i$ for all $i \in N(i_1)$. Since $u_j - u_{i_1} \leq 0$ for each $j \in N(i_1)$, the right-hand side of the previous inequality does not exceed $d_{i_1 i_2}(u_{i_2} - u_{i_1}) + \lambda a(1-a)(u_{i_1} - a)$ and therefore

$$u_{i_2} \geq u_{i_1} - \frac{\lambda}{d_{\min}} a(1-a)(u_{i_1} - a) = a + \varepsilon(1 - L), \tag{3.2}$$

where $L := \frac{\lambda}{d_{\min}} a(1-a)$. If the first inequality in (3.1) holds then $u_{i_2} > a$ which contradicts Lemma 3.2 in the case of $\operatorname{diam}(G) = 1$.

Further, let us assume $\operatorname{diam}(G) > 1$. We consider the k-neighbourhood of i_1 defined by

$$N_k(i_1) = \{j \in V : \operatorname{dist}(i, j) \leq k\}.$$

Let us assume that i_k, $k = 2, 3, \ldots, \operatorname{diam}(G)$ is a vertex where u attains its minimal value on the k-neighbourhoods $N_k(i_1)$ and let us study the lower estimates for u_{i_k} and show via induction that they satisfy $u_{i_k} > a$. Assuming that $u_{i_k} > a$ we show that $u_{i_{k+1}} > a$. We have the following estimate

$$0 = \sum_{j \in N(i_k)} d_{i_k j}\,(u_j - u_{i_k}) + \lambda f(u_{i_k}) \leq \sum_{j \in N(i_k)} d_{i_k j}\,(u_j - u_{i_k}) + \lambda a(1-a)(u_{i_k} - a).$$

Employing the fact that $u_j \leq u_{i_1}$ for all $j \in N(i_k)$ we get:

$$u_{i_{k+1}} \geq u_{i_k} - \frac{d_{\max}}{d_{\min}}(\deg(i_k) - 1)(u_{i_1} - u_{i_k}) - \frac{\lambda}{d_{\min}} a(1-a)(u_{i_k} - a).$$

Since $u_{i_k} - a \leq \varepsilon$ and $u_{i_1} - u_{i_k} = a + \varepsilon - u_{i_k}$, we get

$$u_{i_{k+1}} \geq u_{i_k} - D(a + \varepsilon - u_{i_k}) - L\varepsilon,$$

where $D := \frac{d_{\max}}{d_{\min}}(\Delta(G) - 1)$. Since the solution of the difference equation

$$\begin{cases} x_{k+1} = x_k - D(a + \varepsilon - x_k) - L\varepsilon, \\ x_2 = a + \varepsilon(1 - L). \end{cases}$$

is given by

$$x_k = a + \varepsilon\left(1 - \frac{L}{D}\left((1+D)^{k-1} - 1\right)\right),$$

we get the following estimates for values in i_k

$$u_{i_k} \geq a + \varepsilon\left(1 - \frac{L}{D}\left((1+D)^{k-1} - 1\right)\right).$$

Since $k \leq \operatorname{diam}(G)$ (i.e., each vertex is attainable in at most k steps from i_1), we obtain for all $i \in V$:

$$u_i \geq a + \varepsilon \left(1 - \frac{L}{D}\left((1+D)^{\operatorname{diam}(G)-1} - 1\right)\right)$$

Employing the definitions of L and D and the inequality (3.1) we obtain that $u_i > a$ for all $i \in V$.

Similarly, if $a < \frac{1}{2}$ we can replicate the argument, use the estimate for $s \in (0, a)$

$$f(s) \geq f'(a)(s-a) = a(1-a)(s-a),$$

and start with a vertex $i_1 \in V$ such that $u_{i_1} = a - \varepsilon \leq u_i$ for all $i \in V$ to show that $u_i < a$ for all $i \in V$.

Consequently, Lemma 3.2 yields a contradiction with u being a non-constant solution. □

Remark 3.4. Note that, the case of $\operatorname{diam}(G) = 1$ corresponds to complete graphs $G = K_n$, $n = 2, 3, \ldots$. In this case the condition is simpler because we only consider the one-neighbourhood. The proof shows that if the latter inequality in (3.1) holds (assuming that $\operatorname{diam}(G) > 1$) then the former is also satisfied.

Using the variational structure of the energy functional corresponding to (2.2) we are able to show the following sufficient condition for the existence of non-constant (spatially heterogeneous) solutions. We denote by $\rho(A)$ the spectral radius (i.e., the largest eigenvalue) of the graph Laplacian A.

Theorem 3.5. *Let the inequality*

$$\lambda > \frac{\rho(A)}{a(1-a)} \tag{3.3}$$

hold. Then there exists at least one non-constant stationary solution of (1.5).

Proof. We study the geometry of the energy functional corresponding to (2.2), i.e.,

$$\mathcal{F}(u) = \frac{1}{2}(Au, u) - \sum_{i=1}^{n} g(u_i),$$

where g is the potential to the the reaction function λf

$$g(s) = \lambda \int_0^s f(t)\mathrm{d}t = \frac{\lambda}{12} s^2 \left(-3s^2 + 4s(a+1) - 6a\right).$$

Apparently, $\mathcal{F}(u)$ is weakly coercive since A is positive semidefinite and $g(s) \to -\infty$ as $|s| \to \infty$, i.e.,

$$\mathcal{F}(u) \geq -\sum_{i=1}^{n} g(u_i) \overset{\|u\| \to \infty}{\to} \infty.$$

Consequently, $\mathcal{F}$ also trivially satisfies the Palais-Smale condition, since any sequence (u_n) converging to a critical value $\mathcal{F}(u_n) \to c$, $c \in \mathbb{R}$, must be bounded and contains therefore a convergent subsequence.

First, let us recall that v^1, v^2, v^3 are critical points of $\mathcal{F}$ since they solve (2.2). We show that both $v^1 = o$ as well as $v^3 = e_1 = [1, \ldots, 1]$ are local minima of $\mathcal{F}$. Indeed, the Hessian matrix given by (cf. the proof of Theorem 2.3)

$$H(v^1) = A - \lambda \operatorname{diag}[f'(0), \ldots, f'(0)] = A + \lambda \operatorname{diag}[a, \ldots, a]$$

is positive definite (using the Gerschgorin theorem) and thus $\mathcal{F}$ attains at $v^1 = o$ local minimum. Similarly,

$$H(v^3) = A - \lambda \operatorname{diag}[f'(1), \ldots, f'(1)] = A + \lambda \operatorname{diag}[1-a, \ldots, 1-a]$$

is positive definite and thus $\mathcal{F}$ attains at $v^3 = e_1$ local minimum. Finally, considering the last constant stationary solution $v^2 = ae_1 = [a, \dots, a]$, we observe that the Hessian matrix

$$H(v^2) = A - \lambda \mathrm{diag}[f'(a), \dots, f'(a)] = A - \lambda \mathrm{diag}[a(1-a), \dots, a(1-a)]$$

is a perturbation of positive semidefinite A by a negative definite diagonal matrix $-\lambda a(1-a)I$. We show that under (3.3) the matrix $H(v^2)$ is negative definite. Indeed, we can write

$$(H(v^2)u, u) = ((A - \lambda a(1-a)I)u, u) = (Au, u) - \lambda a(1-a)(u, u).$$

Employing (3.3) we observe that for $u \neq o$

$$(H(v^2)u, u) < (Au, u) - \rho(A)(u, u) \leq 0.$$

Consequently, $H(v^2)$ is negative definite and a local maximum of $\mathcal{F}$ is attained at $v^2 = ae_1 = [a, \dots, a]$ if (3.3) holds.

Furthermore we can compute the exact values of the functional at v^i, $i = 1, 2, 3$. Evaluating the function g

$$g(0) = 0, \quad g(a) = \frac{\lambda a^3}{12}(a-2), \quad g(1) = \frac{\lambda}{12}(1-2a),$$

we get (using the fact that $Au = o$ for constant vectors)

$$\mathcal{F}(v^1) = 0, \quad \mathcal{F}(v^2) = -n\frac{\lambda a^3}{12}(a-2), \quad \mathcal{F}(v^3) = -n\frac{\lambda}{12}(1-2a),$$

which implies that $\mathcal{F}(v^2) > \max\{\mathcal{F}(v^1), \mathcal{F}(v^3)\}$

Next we decompose $\mathbb{R}^N$ into two subspaces, using the eigenvectors of the graph Laplacian A,

$$\mathbb{R}^N = Y \oplus Z, \quad Y = \mathrm{span}\{e_1\}, \quad Z = \mathrm{span}\{e_2, \dots, e_N\}.$$

Let us observe that for any $z \in Z$, $z \neq o$ we have for some $\varepsilon > 0$

$$\mathcal{F}(v^2 + z) > \max\{\mathcal{F}(v^1), \mathcal{F}(v^3)\} + \varepsilon. \tag{3.4}$$

Indeed, let us choose ε so that for all $\|z\| \leq \sqrt{\frac{2\varepsilon}{\lambda_2}}$ the inequality $\mathcal{F}(v^2+z) > \max\{\mathcal{F}(v^1), \mathcal{F}(v^3)\} + \varepsilon$ holds (we can find such ε because $\mathcal{F}(v^2) > \max\{\mathcal{F}(v^1), \mathcal{F}(v^3)\}$). If $\|z\| > \sqrt{\frac{2\varepsilon}{\lambda_2}}$ we get the following estimate

$$\mathcal{F}(v^2+z) = \frac{1}{2}(Az, z) - \sum_{i=1}^{n} g(a+z_i) \geq \frac{1}{2}\lambda_2\|z\|^2 - n\max_{s\in\mathbb{R}} g(s) > \varepsilon - n\max_{s\in\mathbb{R}} g(s) = \max\{\mathcal{F}(v^1), \mathcal{F}(v^3)\} + \varepsilon,$$

where the last equality holds since $\max_{s\in\mathbb{R}} g(s) = g(0) = 0$ for $a \geq 1/2$ or $\max_{s\in\mathbb{R}} g(s) = g(1) = \frac{\lambda}{12}(1-2a)$ if $a < 1/2$. Therefore, the inequality (3.4) holds and we observe immediately that

$$\inf_{z\in Z} \mathcal{F}(v^2+z) \geq \varepsilon - n\max_{s\in\mathbb{R}} g(s) = \max\{\mathcal{F}(v^1), \mathcal{F}(v^3)\} + \varepsilon.$$

Consequently, we can apply the saddle point theorem (see, e.g., [23, Theorem 4.6]) to prove that there exists another critical point u^* (with a saddle point geometry) of the functional $\mathcal{F}$. The a priori estimate Lemma 3.1 yields that $u^* \in [0, 1]^n$. □

Remark 3.6.
- In Section 5 we provide a simple example of a complete graph with two vertices $G = K_2$ that shows that the sufficient condition (3.3) is also necessary in some special cases. However, for general graphs, this estimate could be improved.

- Combining Theorems 3.3 and 3.5, we get bounds for $\underline{\lambda}$, see Figure 1. For example, for complete graphs K_n with constant diffusion $d = d_{ij}$ along the edges we obtain:

$$\frac{d}{a(1-a)} \le \underline{\lambda} \le \frac{2d}{a(1-a)}.$$

- In general, there exist multiple estimates on the spectral radius $\rho(A)$. The simplest one comes from the application of the Gerschgorin theorem and implies that $\rho(A) \le 2d_{\max}\Delta(G)$. More intricate ones usually assume constant diffusion along the edges $d_{ij} = d$. Then we can for example prove that $\rho(A) \le d \cdot \max\{\deg(u) + \deg(v), (u,v) \in E\}$, for other estimates see e.g. [17].

- If $a = 1/2$ the symmetry immediately implies that there are at least two non-constant stationary solutions. For $a \ne 1/2$ this remains open, even if numerical experiments indicate that it is also true (see Section 5). Finally, note that the right-hand side of the sufficient condition (3.3) tends to infinity as $a \to 0+$ or $a \to 1-$.

4 Exponential number and stability of non-constant stationary solutions

In this section we show that, for large values of λ, the number of non-constant (spatially heterogeneous) stationary solutions rises exponentially and identify their stability. If we rewrite (2.2) as $o = -\frac{1}{\lambda}Au + F(u)$ and observe that $f(s) = 0$ has three roots, we can expect to get 3^n solutions for large values of λ.

Theorem 4.1. *Let*

$$\lambda > \frac{4 \cdot d_{max} \cdot \Delta(G)}{\min\{a^2, (1-a)^2\}}. \tag{4.1}$$

Then there exist at least 3^n stationary solutions of the graph reaction-diffusion equation (1.5).

Proof. First, let us show that for sufficiently large λ there are 3^n stationary solutions. For given a and λ we define a vector $s \in \{0, a, 1\}^n$. Apparently, there are 3^n such vectors. For each s we define an operator $T_s : [0,1]^n \to [0,1]^n$ by

$$T_s(x) := (\tau_1(s_1, x), \tau_2(s_2, x), \dots, \tau_n(s_n, x)), \tag{4.2}$$

where the functions $\tau_i : \{0, a, 1\} \times [0,1] \to [0,1]$ are defined by

$$\tau_i(s_i, x) := \begin{cases} r_{i,1} & \text{if } s_i = 0, \\ r_{i,2} & \text{if } s_i = a, \\ r_{i,3} & \text{if } s_i = 1, \end{cases}$$

and $r_{i,j}$, $j = 1, 2, 3$, are the roots of the cubic function

$$\varphi_i(u) := \sum_{j \in N(i)} d_{ij}(x_j - u) + \lambda u(u-a)(1-u), \tag{4.3}$$

ordered by $0 \le r_{i,1} < r_{i,2} < r_{i,3} \le 1$. The fact that there are three distinct roots $r_{i,j}$, $j = 1, 2, 3$, lying between 0 and 1 follows from the following estimate

$$\underline{\varphi_i}(u) \le \varphi_i(u) \le \overline{\varphi_i}(u), \tag{4.4}$$

where

$$\underline{\varphi_i}(u) := -\Delta(G) d_{max} u + \lambda u(u-a)(1-u),$$
$$\overline{\varphi_i}(u) := \Delta(G) d_{max}(1-u) + \lambda u(u-a)(1-u).$$

The roots of the cubic lower estimate $\underline{\varphi_i}(u)$ are

$$0, \frac{1}{2}\left(1+a \pm \sqrt{(1-a)^2 - \frac{4\Delta(G)d_{max}}{\lambda}}\right), \tag{4.5}$$

and the roots of the cubic upper estimate $\overline{\varphi_i}(u)$ are

$$1, \frac{1}{2}\left(a \pm \sqrt{a^2 - \frac{4\Delta(G)d_{max}}{\lambda}}\right). \tag{4.6}$$

If λ satisfies (4.1) then the discriminants in (4.5)-(4.6) are positive and the roots are distinct and located in $[0,1]$. Consequently, the estimate (4.4) implies that the three distinct roots of $\varphi_i(u)$ satisfy $0 \leq r_{i,1} < r_{i,2} < r_{i,3} \leq 1$ and the operator T_s (4.2) is well-defined. Apparently, the operator T_s is continuous since the roots of cubic functions depend continuously on the cubic polynomials' coefficients. Consequently, the Brouwer fixed-point (e.g., [10, Theorem 5.1.3]) theorem yields that T_s has a fixed point in $[0,1]^n$.

The definition of T_s (4.2) implies that there are 3^n distinct operators. Each of them has a different fixed point. Indeed, let us assume by contradiction that $s, \sigma \in \{0, a, 1\}^n$ with $s \neq \sigma$ generate operators T_s and T_σ with an identical fixed point, i.e. there exists x^* such that $T_s(x^*) = T_\sigma(x^*) = x^*$. The contradiction follows immediately from the fact that $\tau_i(s_i, x) \neq \tau_i(\sigma_i, x)$ whenever $s_i \neq \sigma_i$.

Finally, we observe that the fixed point of each T_s is a stationary solution of (2.1). Indeed, if $x \in [0,1]^n$ is a fixed point of T_s given by (4.2) then the definition of φ_i (4.3) implies that for all $i \in V$:

$$\varphi_i(x_i) = \sum_{j \in N(i)} d_{ij}(x_j - x_i) + \lambda x_i(x_i - a)(1 - x_i) = 0,$$

which yields that $x \in [0,1]^n$ is a stationary solution of (1.5). Therefore, there are at least 3^n stationary solutions of (2.1). ☐

Remark 4.2. The main contribution of Theorem 4.1 is the lower estimate (4.1). Alternatively, we could arrive to a similar conclusion by applying the implicit function theorem for the equation $o = \varepsilon Au + F(u) = -\frac{1}{\lambda}Au + F(u)$ at $\varepsilon = 0$ (note that we have a finite dimension and A is a matrix, i.e., a bounded operator). This approach yields no lower estimate of the type (4.1) but on the other hand provides the existence of exactly 3^n solutions (note that $F(u) = o$ has exactly 3^n solutions). Such an approach via the implicit function theorem has been used for lattice differential equations e.g. in [15, 22] whereas our approach is closer to Keener's approach [13].

Finally, we show that if λ is sufficiently large there exist 2^n asymptotically stable stationary solutions.

Theorem 4.3. *There exists $\tilde{\lambda}$ such that for all $\lambda > \tilde{\lambda}$ there are 2^n asymptotically stable stationary solutions of* (1.5).

Proof. It remains to prove that there are 2^n asymptotically stable stationary solutions. Let x_s be the fixed point of T_s defined in (4.2) with $s \in \{0,1\}^n$ and, consequently, the stationary solution of (2.1). The stability of this solution is given by the eigenvalues of

$$-A + \lambda F'(x_s).$$

Since the graph Laplacian A is positive semidefinite, it is enough to show that the diagonal matrix $F'(x_s)$ contains only negative entries $f'((x_s)_i)$ on the diagonal. Thus, we need to show that $f'((x_s)_i) = (2 - 3(x_s)_i)(x_s)_i + a(-1 + 2(x_s)_i) < 0$. Since $f(u)$ is a cubic function with $f(u) \to -\infty$ as $u \to +\infty$ it is enough to show that $(x_s)_i$ is either greater or smaller than both local extrema u_1 and u_2 of $f(u)$ (we assume that $u_1 < u_2$). Since (4.4) holds, it suffices to prove that u_2 is smaller than the largest zero of

$\underline{\varphi_i}(u)$, because $(x_s)_i$ must be greater than the largest zero of $\underline{\varphi_i}(u)$ and $f'(u) < 0$ for all $u > u_2$. Thus, see (4.5),

$$u_2 = \frac{1}{3}\left(1 + a + \sqrt{1 - a + a^2}\right) < \frac{1}{2}\left(1 + a + \sqrt{(1-a)^2 - \frac{4\Delta(G)d_{max}}{\lambda}}\right),$$

and, simultaneously, u_1 greater than the smallest zero of $\overline{\varphi_i}(u)$, i.e. (see (4.6)),

$$u_1 = \frac{1}{3}\left(1 + a - \sqrt{1 - a + a^2}\right) > \frac{1}{2}\left(a - \sqrt{a^2 - \frac{4\Delta(G)d_{max}}{\lambda}}\right).$$

Expressing λ from the former expression we get that

$$\lambda > \tilde{\lambda}_1 := \frac{\left(a\left(-a + \sqrt{(a-1)a+1} + 4\right) + \sqrt{(a-1)a+1} - 1\right)\Delta(G)d_{max}}{(a-1)^2 a},$$

and, repeating the procedure for the latter inequality, we require at the same time,

$$\lambda > \tilde{\lambda}_2 := \frac{\left(a\left(a + \sqrt{(a-1)a+1} + 2\right) - 2\left(\sqrt{(a-1)a+1} + 1\right)\right)\Delta(G)d_{max}}{(a-1)a^2}.$$

Consequently, if λ satisfies

$$\lambda > \tilde{\lambda} := \max\{\tilde{\lambda}_1, \tilde{\lambda}_2\},$$

we have that $F'(x_s)$ is a negative diagonal matrix and hence the matrix $-A + \lambda F'(x_s)$ is negative definite which implies that every x_s with $s \in \{0,1\}^n$ is asymptotically stable. □

Remark 4.4. First, note that $\tilde{\lambda} > \frac{4 \cdot d_{max} \cdot \Delta(G)}{\min\{a^2,(1-a)^2\}}$. Comparing $\tilde{\lambda}$ and $\frac{4 \cdot d_{max} \cdot \Delta(G)}{\min\{a^2,(1-a)^2\}}$ we observe that for $a \in [1/2, 1)$

$$\begin{aligned}\tilde{\lambda} - \frac{4 \cdot d_{max} \cdot \Delta(G)}{\min\{a^2,(1-a)^2\}} &= \tilde{\lambda}_1 - \frac{4 \cdot d_{max} \cdot \Delta(G)}{a^2} \\ &= \frac{1}{a\left(a + \sqrt{(a-1)a+1}\right) + \sqrt{(a-1)a+1} + 1}\Delta(G)d_{max} > 0,\end{aligned}$$

and a similar inequality holds for $a \in (0, 1/2]$.

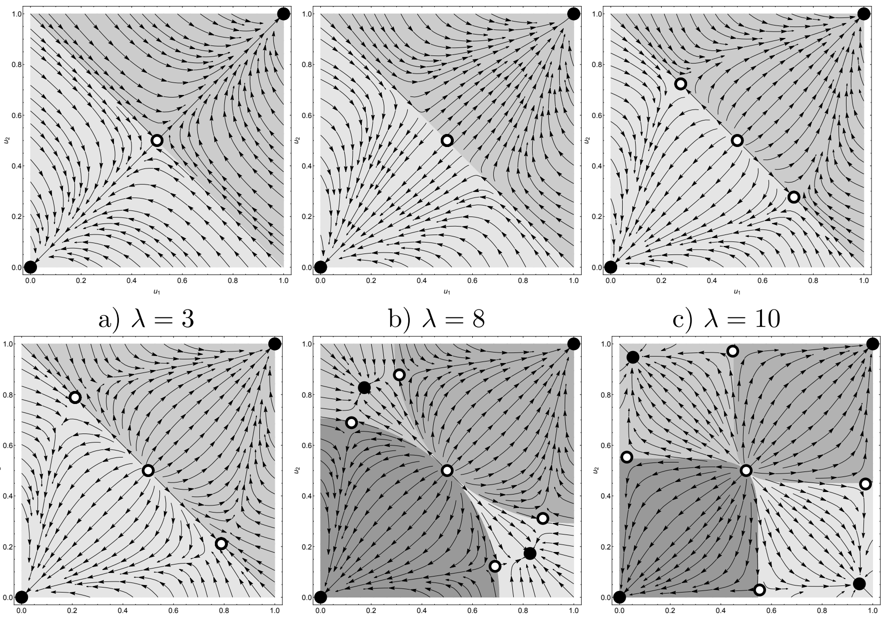
In the following section, we study analytically the behaviour of the reaction-diffusion equation on the simple graph $G = K_2$ and show that assumptions of Theorems 4.1 and 4.3 are far from being optimal. Note that the bound (4.1) corresponds exactly to the Keener's estimate for one-dimensional lattice of [13, Theorem 2.8]) and the condition on stability (Theorem 4.3 improves the estimate implied by [13, Corollary 2.2].

5 Example

In this section we illustrate our results on a trivial example and discuss optimality of assumptions on λ. In order to be able to compute everything analytically, let us focus on the simplest possible configuration. Let us consider $G = K_2$ and assume that $d = 1$ and $a = \frac{1}{2}$. Then the graph RDE (1.5) reduces to the system of two ODEs

$$u_1'(t) = (u_2(t) - u_1(t)) + \lambda u_1(t)\left(u_1(t) - \frac{1}{2}\right)(1 - u_1(t)) \tag{5.1}$$

$$u_2'(t) = (u_1(t) - u_2(t)) + \lambda u_2(t)\left(u_2(t) - \frac{1}{2}\right)(1 - u_2(t)) \tag{5.2}$$



a) $\lambda = 3$ b) $\lambda = 8$ c) $\lambda = 10$

d) $\lambda = 12$ e) $\lambda = 14$ f) $\lambda = 40$

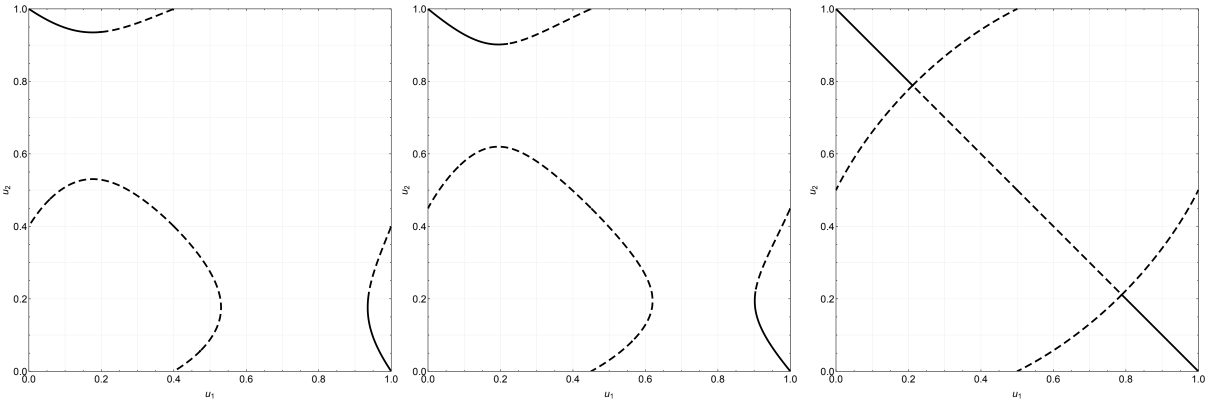
Figure 3: Spatially nonhomogeneous stationary solutions of the graph RDE for $G = K_2$, see (5.1)-(5.2), their stability (full discs correspond to asymptotically stable solutions, empty discs to unstable ones) and their basins of attraction for various values of λ.

In this case the graph Laplacian has the form $A = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$, its eigenvalues are $\lambda_1 = 0$ and $\lambda_2 = 2$. Thus, $\rho(A) = 2$. Observing (5.1)-(5.2) and using substitution one can find all stationary solutions by finding roots of a ninth order polynomial. Its analysis yields that

- $0 < \lambda < 8$ - there are three simple real roots, corresponding to $[0, 0]$, $[1/2, 1/2]$ and $[1, 1]$, and 6 complex ones,
- $\lambda = 8$ - there are still three roots, but the multiplicty of $[1/2, 1/2]$ becomes three, two new solutions bifurcate,
- $8 < \lambda < 12$ - there are five simple real roots $[0, 0]$, $[1/2, 1/2]$ and $[1, 1]$ and $[\alpha, \beta]$, $[\beta, \alpha]$ with $\alpha \in (0, 1/2)$ and $\beta \in (1/2, 1)$,
- $\lambda = 12$ - there are still five real roots, but the multiplicty of $\left[\frac{1}{6}\left(3 - \sqrt{3}\right), \ \frac{1}{6}\left(3 + \sqrt{3}\right)\right]$, $\left[\frac{1}{6}\left(3 + \sqrt{3}\right), \ \frac{1}{6}\left(3 - \sqrt{3}\right)\right]$ becomes three,
- $\lambda > 12$, - there are nine real roots.

As predicted by the proof of Theorem 4.1, as $\lambda \to \infty$ the nine solutions tend to the nine limits $\{0, 1/2, 1\}^2$. The stability analysis shows that for $\lambda > 12$ the four solutions lying on branches tending to $\{0, 1\}^2$ are asymptotically stable, the remaining five solutions are unstable (see Theorem 4.3). The dependence on λ and the stability of non-constant stationary solutions are visualised in Figure 3 and aggregately in Figure 4, panel c).

Let us discuss the optimality of assumptions of our results. In the case of $G = K_2$, we observe that the assumption (3.3) of Theorem 3.5 on the existence on non-constant stationary solutions is optimal in



a) $a = .4$ b) $a = .45$ c) $a = .5$

Figure 4: Location of spatially nonhomogeneous stationary solutions of the graph RDE for $G = K_2$, see (5.1)-(5.2) for various values of a, their stability is indicated by full lines and their instability by dashed lines. Each picture shows locations of non-constant solutions for all $\lambda > 0$, cf. Figure 3 with panel c).

this cases since a simple computation yields

$$\lambda > \frac{\rho(A)}{a(1-a)} = 8.$$

This is also true for other complete graphs. However, note that this is no longer true if we consider other graphs (see Conjecture 6.2). The sufficient condition for the nonexistence (3.1) is not optimal since it only predicts the nonexistence for $\lambda < 4$. Similarly, the sufficient conditions for the existence of exponential number of stationary solutions (see Theorems 4.1 and 4.3) are not optimal and could apparently be improved. The sufficient conditions of Theorem 4.1 only yield that 3^n solutions exist if $\lambda > 16$ and Theorem 4.3 provides that 2^n out of these solutions are asymptotically stable if $\lambda > 6(1+\sqrt{3}) \approx 16.39$.

Similar procedures could be repeated numerically for values of $a \neq 1/2$. Theorem 3.5 indicates that spatially nonhomogeneous solutions bifurcate from (a, a) at $\lambda = \frac{2}{a(1-a)}$. This behaviour is similar to the case $a = 1/2$. However, in the asymmetrical case the branches of non-constant solutions do not occur via the subcritical pitchfork bifurcation but we observe saddle-node bifurcations (cf. Figure 4).

6 Final remarks and open problems

Our analysis has revealed an interesting relationship between the reaction-diffusion dynamics and graph-theoretical properties. Firstly, we provided bounds for the existence of non-constant (spatially heterogeneous) stationary solutions of the graph Nagumo equation. Theorems 3.3 and 3.5 imply that for complete graphs we have

$$\frac{d_{\min}}{a(1-a)} \leq \underline{\lambda} \leq \frac{\rho(A)}{a(1-a)}. \tag{6.1}$$

Our numerical experiments suggest that $\underline{\lambda} = \frac{\lambda_2}{a(1-a)}$, where λ_2 is the second eigenvalue of the graph Laplacian A. For example, the upper bound in (6.1) is optimal for complete graphs $G = K_n$, $n \in \mathbb{N}$ for which we have $\rho(A) = \lambda_2$. The lower bound (3.1) is not optimal even in special cases.

Conjecture 6.1. There exist no spatially heterogeneous stationary solutions for $\lambda \leq \frac{\lambda_2}{a(1-a)}$.

One could show, using the Krasnoselski local bifurcation theorem, that $\frac{\lambda_2}{a(1-a)}$ is a point of bifurcation of spatially heterogeneous stationary solutions from the unstable constant solution $(a, a, \dots, a)$. However, this could be done only for the cases when λ_2 has odd multiplicities and the theorem does not ensure existence of non-constant stationary solutions for all $\lambda > \frac{\lambda_2}{a(1-a)}$.

Conjecture 6.2. There exists at least one spatially heterogeneous stationary solution for $\lambda > \frac{\lambda_2}{a(1-a)}$.

Once $\lambda > \underline{\lambda}$ we enter the transition region where non-constant stationary solutions bifurcate in a very intricate way, see Figure 1. At this stage we are far from being able to describe this process fully for a general graph G as in the case of $G = K_2$, see Section 5 and Figures 3-4. However, numerical experiments indicate some simple connection to the parameters of the problem.

Conjecture 6.3. *The number of stationary solutions of (1.5) is nondecreasing in λ and nonincreasing in d_{ij} for all $(i,j) \in E$.*

The next conjecture is also linked to the number of solutions but this time associated with the shape of the bistable nonlinearity.

Conjecture 6.4. The number of stationary solutions of (1.5) is nonincreasing in $|a - 1/2|$.

Naturally, the most interesting relationship involves the graph structure and various graph properties. For example, let us fix the number of vertices. Numerical experiments indicate that the occurrence of non-constant stationary solutions is closely connected to the number of edges of the graph. In principle, the weaker reaction (i.e., smaller λ) is sufficient for the occurrence of non-constant stationary solutions on sparser graphs.

Conjecture 6.5. Let $\lambda > 0$, G be a graph and G' be a graph obtained from G by adding an edge. If there exists a non-constant solution of (1.5) on G' then there exists a non-constant solution of (1.5) on G as well.

Conjecture 6.6. Let $\lambda > 0$, G be a graph and G' be a graph obtained from G by adding an edge. If there exist 3^n stationary solutions of (1.5) on G' then there exist 3^n stationary solutions of (1.5) on G as well.

Note that the conjecture is trivially valid for large values of λ (see Remark 4.2). The interesting part is whether this is true for any λ. Also note that if we add an edge to a graph then the lower estimate in (4.1) either remains the same or increases.

Finally, there is a natural goal to improve the sufficient condition for the existence of 3^n stationary solutions and 2^n asymptotically stable stationary solutions. Recall that the our estimate from Theorem 4.1, i.e., $\overline{\lambda} < \frac{4 \cdot d_{max} \cdot \Delta(G)}{\min\{a^2, (1-a)^2\}}$, is far from optimal even in the simplest example of $G = K_2$, see Section 5. We do not even have a conjecture for the exact value of $\overline{\lambda}$ as in the case of $\underline{\lambda}$, see Conjecture 6.2. In the same spirit, we have not even been able to prove the following conjecture unless we restrict ourselves to the case $\lambda \to \infty$, see Remark 4.2.

Conjecture 6.7. The problem (1.5) has 3^n stationary solutions if and only if it has got 2^n asympotically stable stationary solutions.

More broadly, note that a large part of our paper considered the problem of finding the stationary solution (2.2). The nonlinear algebraic equations have been studied recently by many authors and via various techniques, e.g., [11, 19, 20, 28]. We believe that applications of some of these techniques could improve our estimates. On the other hand, the connection with the graph structures could increase motivation in the study of nonlinear algebraic equations and provide some interesting relationships (e.g., via the eigenvalue properties of the graph Laplacian).

Finally, it would be interesting to see how some other properties from the regular lattices could be carried over to other classes of (possibly infinite) graphs, e.g., the existence of travelling waves [8, 12, 13] or the dependence on the timing structure or other types of partial differential equations on graphs [12, 25, 26].

Acknowledgements

The author gratefully acknowledges the support by the Czech Science Foundation, grant no. GA15-07690S. He also thanks gratefully to Antonník Slavík and Jonáš Volek for their help and valuable discussions. Finally, the author is grateful to two anonymous referees for their detailed and helpful comments.

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